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Multimedia Fate and Transport Models
An Overview

(U.S.) Environmental Research Lab., Athens, GA

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16. ABSTRACT

This paper examines the development and current status of several multimedia fate and transport models that are designed for application to specific single pollutants and for general purpose evaluation of toxic chemicals. The capabilities, limitations, and data requirements of these models are briefly reviewed.

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MULTIMEDIA FATE AND TRANSPORT MODELS: AN OVERVIEW

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Models of the environmental fate and transport of chemicals are used to predict pollutant concentrations in air, land, and water for exposure and risk assessment purposes. Although some are relatively advanced, such models typically consider only the fate of the released compound in a single medium (air, water, soil, etc.). To predict adequately the environmental concentrations of many chemicals, however, more than one transport medium must be considered simultaneously, i.e., multimedia modeling must be used. This paper examines the development and current status of multimedia fate and transport models designed for application to specific, single pollutants and for general purpose evaluation of toxic chemicals.

The concepts for risk and exposure assessments used here (Figure 1) were developed during the Predictive Exposure Assessment Workshop sponsored by the U.S. Environmental Protection Agency in Atlanta, Georgia, on April 27-29, 1982.

According to these concepts, to make an exposure assessment,

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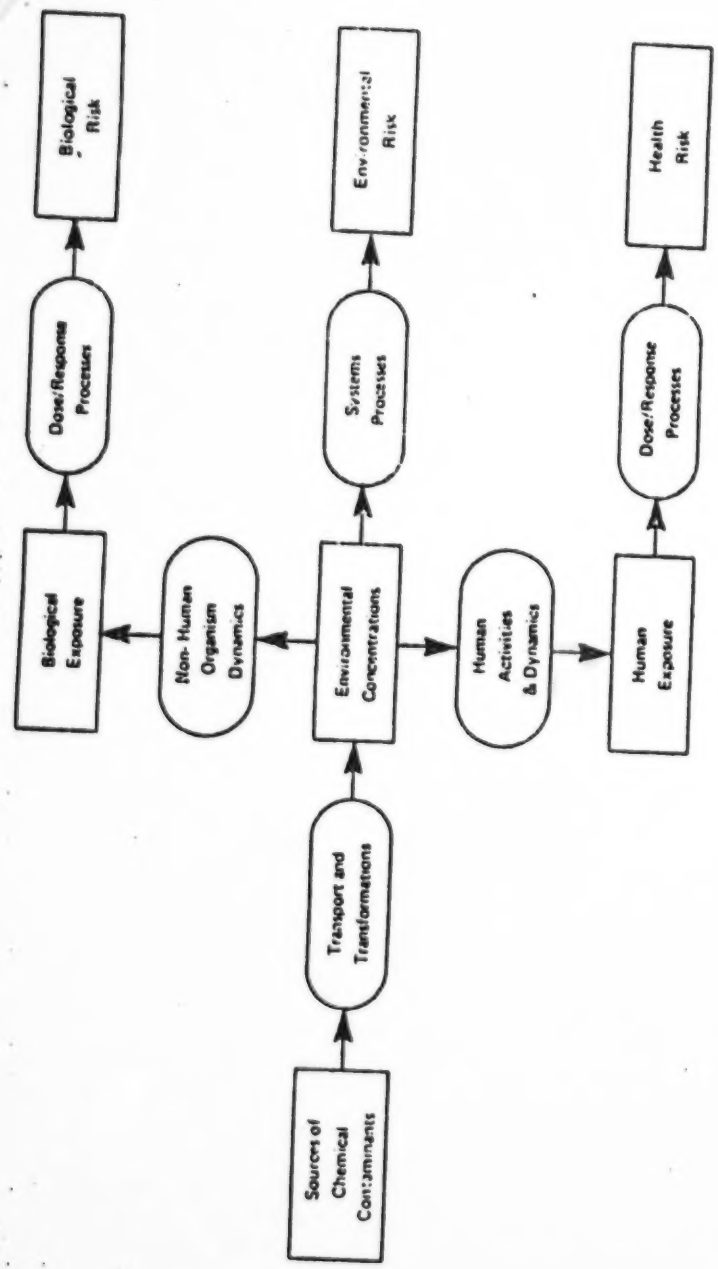

FIGURE 1
Concepts for Risk and Exposure Assessment

analysts need information about the amounts of chemical being released (loads), the characteristics of the receiving environment, the processes that modify or move the chemical through that environment, and the activities and dynamics of the population being exposed (receptor population). This paper will focus only on multimedia models that predict environmental concentrations.

Figure 2 shows the representative pathways a pollutant can take to reach a human population (1). It can be seen that by various processes, pollutants can undergo intermedia transfer following their initial appearance in soil, surface water, ground water, and air.

Several global models for specific pollutants were developed in the late 1960s and early 1970s. Along with more recent global models, they are primarily useful for natural resource policy analysis on a national or regional scale rather than for exposure or risk assessments (2).

Intermedia transport models have been developed for toxic trace metals and for organic chemicals. They are either dynamic (time varying) or steady state (time independent). They vary in terms of the confidence with which each process can be described. The following two levels of modeling within all media are of current regulatory interest:

- Screening (non-site-specific)--Modeling using far-field models. Normally applied when very little information is known about the source site, the chemical (beyond its name and structure), and a general description of the receiving environment. Expected accuracy is within one order of magnitude.

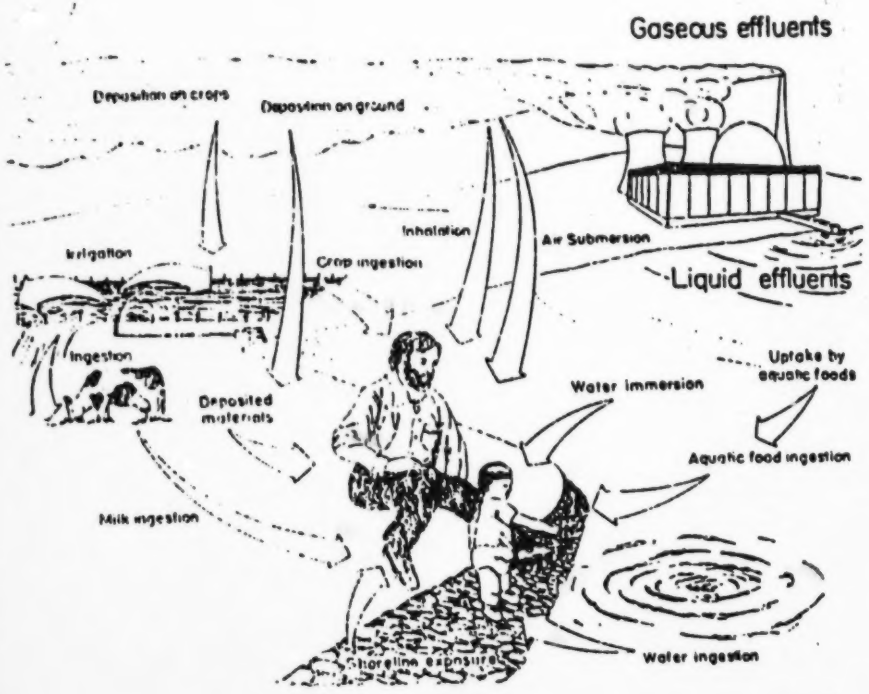

FIGURE 2
Exposure Pathways to Man
From Reference 1

- Site-Specific--Modeling more detailed; requires detailed information about the site, its meteorology, and the physicochemical properties and release characteristics of the emitted pollutant. Expected accuracy is within a factor of two to four for many situations.

Several simple, generic screening models have also been developed. Many are based on simple equilibrium partitioning of the pollutant among the various media; others use more sophisticated, kinetic approaches but with simplified rate

equations and conditions that assume a steady-state operation.

TRACE METALS MODEL

One of the first multimedia models with intermedia transfer processes for specific chemicals (metals) was the Unified Transport Model (UTM) developed by Oak Ridge National Laboratory (3). The UTM simulates the transport of toxic trace metals through an ecosystem consisting of the atmosphere, land surface, vegetation, soil layers, ground water, and streams. It operates with a time step of one hour when rain is absent and 15 minutes when it rains. The UTM is actually a group of models (Figure 3) that may be arranged in different ways so that the output of one serves as input to the next. Different arrangements of these models have been applied to watersheds ranging in size from about 200 hectares to approximately 10,000 square kilometers. When incorporated as part of the UTM, the Atmospheric Transport Model (ATM) limits a study area to a circle of about 70-80 km radius.

The data required by the various arrangements of the specific models in the UTM include historical values of hourly precipitation; daily average wind speed, maximum and minimum temperature, dew point, and total radiation; and values characterizing the watershed topography, soil characteristics, and vegetative cover. (If the ATM is not used, hourly wetfall and monthly dryfall contaminant values are needed. If it is used, then data on the source characteristics, pollutant physical characteristics, and hourly wind speed and direction are also needed.)

Application of the UTM to specific watershed problems

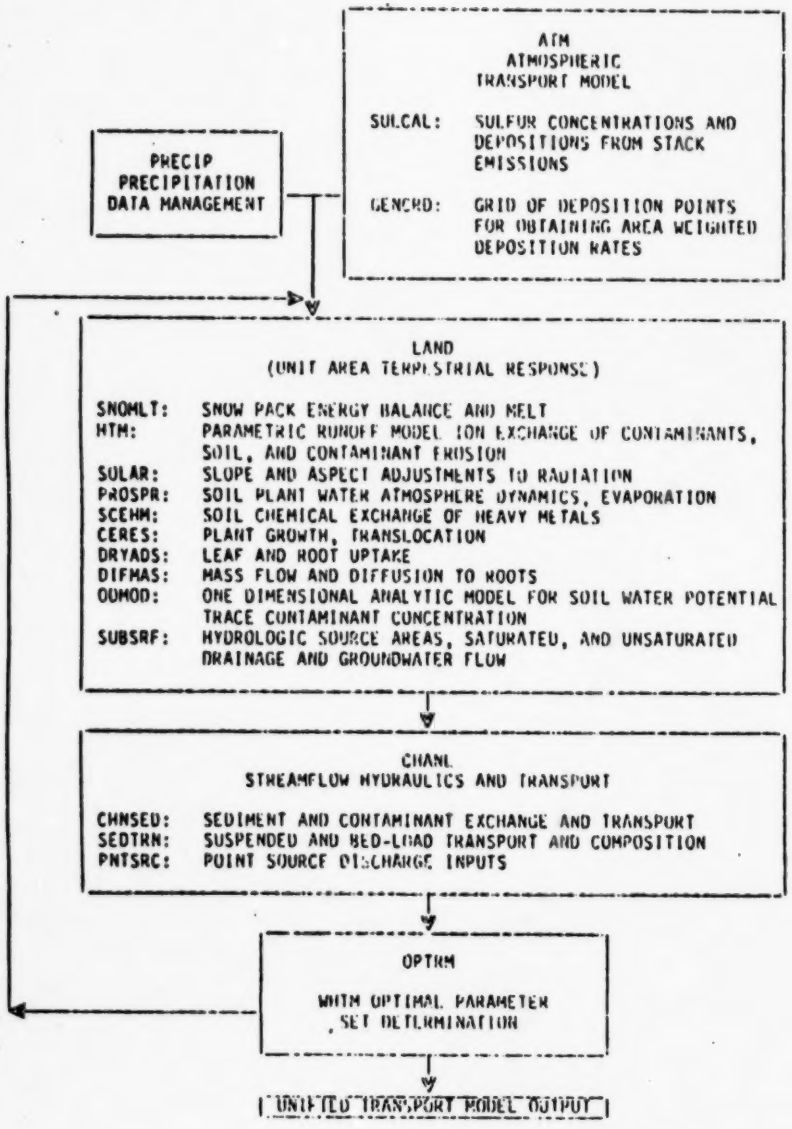
ATM
ATMOSPHERIC
TRANSPORT MODEL
SULCAL: SULFUR CONCENTRATIONS AND DEPOSITIONS FROM STACK EMISSIONS
GENGRD: GRID OF DEPOSITION POINTS FOR OBTAINING AREA WEIGHTED DEPOSITION RATES
PRECIP
PRECIPITATION
DATA MANAGEMENT
LAND
(UNIT AREA TERRESTRIAL RESPONSE)
SNOMLT: SNOW PACK ENERGY BALANCE AND MELT
HTM: PARAMETRIC RUNOFF MODEL ION EXCHANGE OF CONTAMINANTS, SOIL, AND CONTAMINANT EROSION
SOLAR: SLOPE AND ASPECT ADJUSTMENTS TO RADIATION
PROSPR: SOIL PLANT WATER ATMOSPHERE DYNAMICS, EVAPORATION
SCEHM: SOIL CHEMICAL EXCHANGE OF HEAVY METALS
CERES: PLANT GROWTH, TRANSLOCATION
DRYADS: LEAF AND ROOT UPTAKE
DIFMAS: MASS FLOW AND DIFFUSION TO ROOTS
OUMOD: ONE DIMENSIONAL ANALYTIC MODEL FOR SOIL WATER POTENTIAL TRACE CONTAMINANT CONCENTRATION
SUBSRF: HYDROLOGIC SOURCE AREAS, SATURATED, AND UNSATURATED DRAINAGE AND GROUNDWATER FLOW
CHANL
STREAMFLOW HYDRAULICS AND TRANSPORT
CHNSED: SEDIMENT AND CONTAMINANT EXCHANGE AND TRANSPORT
SEDTRN: SUSPENDED AND BED-LOAD TRANSPORT AND COMPOSITION
PNTSRC: POINT SOURCE DISCHARGE INPUTS
OPTRM
WHTM OPTIMAL PARAMETER SET DETERMINATION
UNIFIED TRANSPORT MODEL OUTPUT

FIGURE 3
The Submodels That May Be Linked to Form
a Unified Transport Model
From Reference 3

requires specification of the nature of the information desired, as well as of the available data. The optimal arrangement of the various models in the UTM depends on this information. Appropriate model configuration depends on the nature of the desired simulation; collecting and assembling the required data is always a major effort.

When modeling problems involve air, water, and ground transport, the UTM can be arranged in two ways known as the Wisconsin Hydrologic Transport Model (WHTM) and the Terrestrial Ecosystem Hydrology Model (TEHM). The WHTM is composed of a land and channel segment and can be run using daily values of evaporation. The TEHM, on the other hand, computes evapotranspiration (evaporation and transpiration as a single process) from daily average values of wind speed, mean dew point temperature, and integrated incoming solar radiation. The two arrangements of the UTM differ only in the land simulation portion of the hydrologic component. Figure 4 illustrates requirements and output data for the ATM and WHTM.

WHTM

The WHTM is based on the Stanford Watershed Model, as are the hydrologic components of the other site-specific models to be discussed below. It requires considerably fewer data than TEHM to simulate water quality in streams and buildup of toxic substances in the soil. It also allows for intercepting, storing, and leaching of pollutants from the litter layer.

ATMOSPHERIC TRANSPORT MODEL

INPUT: Type of material (particle or gas), density, size, wind speeds, wind directions, atmospheric stability, geographic location, type and strength of emission sources, height of stack, plume rise factor, hourly precipitation

OUTPUT: Wet and dry deposition amounts, surface concentration

WISCONSIN HYDROLOGIC TRANSPORT MODEL

INPUT: Hourly precipitation, daily maximum and minimum temperatures, daily pan evaporation rates, hourly temperature and humidity, daily precipitation, solar radiation; upper and lower zone soil storage, soil moisture evaporation index, time distribution parameter for interflow, average length of overland flow, average slope of overland flow plane, interflow recession constant, ground water recession parameter, impervious area and other parameters describing land features; residual toxicant mass distributed on land surface, ion-exchange distribution coefficient, deposition amounts, toxicant content of ion exchange plates and other parameters describing toxicant properties.

OUTPUT: Daily stream flow, total metal transported, daily average metal concentration.

FIGURE 4
Input Requirements and Output Data for
Two Components of the Unifed Transport Model
From Reference 3

Evaporation and transpiration are treated together as a single process. The soil profile is divided into surface, upper zone, lower zone, and groundwater. The groundwater storage volume has active and inactive components with the inactive volume assumed to be an infinite sink or source that can be used to allow for water leaving or entering the watershed.

Material transport is treated as a part of the hydrologic flow. The surface soil is represented by a stack of four theoretical ion-exchange plates--the top inch of the upper zone is singled out as the boundary of transition from soil surface to subsurface processes. The pollutant mass is assumed to be mixed uniformly throughout any storage volume and the same ion-exchange distribution coefficient values are assumed to hold for each storage volume where mixing of soil and pollutant occurs.

Surface erosion and transport are treated in terms of thresholds for resuspension of loose soil particles and for erosion of new material. Erosion is driven by the force of water moving over the ground surface. Exchange of pollutants can occur between the surface water and sediments so the discharge to the streams includes water, eroded sediments, amounts of pollutants sorbed on these sediments, and pollutants dissolved in the water.

Once the material discharged from the land surface enters the stream, it is carried through the stream network, with the appropriate timing, to the watershed outfall. The total amount of pollutant entering the stream is used for the channel routing calculations, so that stream concentrations at the outfall include

pollutants both dissolved in the water and sorbed on sediments.

TEHM

The TEHM was specifically developed to emphasize the relationships between plants and their environment (4). Mechanistic models for the soil-plant-water-solute relationships are used as much as the basic UTM arrangement will permit. Compared to the WHTM, the TEHM version presents a more modular treatment of the soil-water processes and allows for a variable number of soil layers of varying characteristics. As a consequence, it also requires substantively more data about the characteristics of the soil and the vegetation. The Soil Chemistry Model (SCEHM) is part of this modular arrangement of the UTM. It is more general than its counterpart in the WHTM arrangement because it allows for varying the values of the ion-exchange distribution coefficients of the soil layers. Pollutant transfer from the soil surface to subsoil, modeled by means of a stack of theoretical ion-exchange plates, is not part of the TEHM, nor is surface erosion.

Figure 5 shows the coupling of the various modules in the TEHM. Atmosphere plant-soil moisture relations are simulated by PROSPR, and the plant water potentials generated are then used by CERES, the submodel that simulates plant growth and respiration: standing crop biomass of leaves, stems, fruits, and roots and storage pools of sugars, live tissue, and dead or woody tissue. CERES also computes the translocation of carriers (transpired water and phloem sugar movement) of chemical substances.

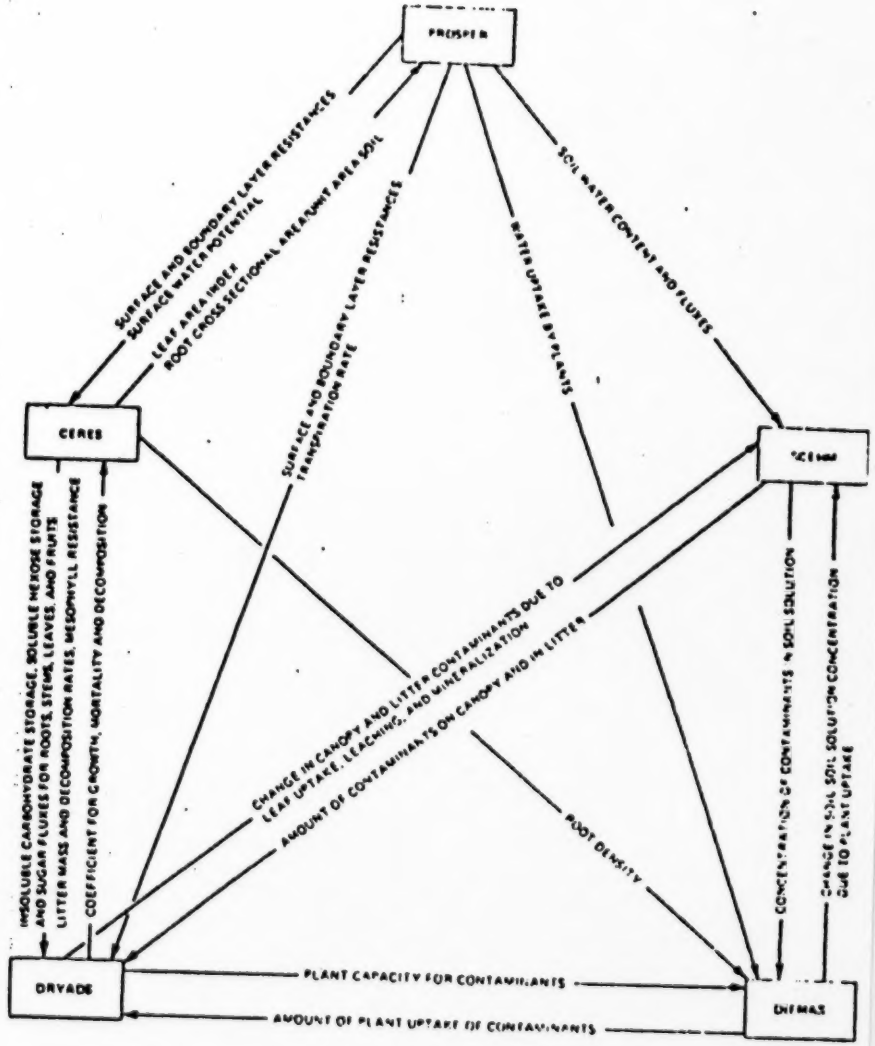
PROSPR
CERES
SCEHM
DRYADS
DEMAS
SURFACE AND BOUNDARY LAYER RESISTANCES
SURFACE WATER POTENTIAL
LEAF AREA INDEX
ROOT CROSS SECTIONAL AREA/UNIT AREA SOIL
SURFACE AND BOUNDARY LAYER RESISTANCES
TRANSPIRATION RATE
WATER UPTAKE BY PLANTS
SOIL WATER CONTENT AND FLUXES
INSOLUBLE CARBOHYDRATE STORAGE, SOLUBLE HEXOSE STORAGE AND SUGAR FLUXES FOR ROOTS, STEMS, LEAVES, AND FRUITS
LITTER MASS AND DECOMPOSITION RATES, MESOPHYLL RESISTANCE
COEFFICIENT FOR GROWTH, MORTALITY AND DECOMPOSITION
CHANGE IN CANOPY AND LITTER CONTAMINANTS DUE TO LEAF UPTAKE, LEACHING, AND MINERALIZATION
AMOUNT OF CONTAMINANTS ON CANOPY AND IN LITTER
ROOT DENSITY
CONCENTRATION OF CONTAMINANTS IN SOIL SOLUTION
CHANGE IN SOIL SOLUTION CONCENTRATION DUE TO PLANT UPTAKE
PLANT CAPACITY FOR CONTAMINANTS
AMOUNT OF PLANT UPTAKE OF CONTAMINANTS

FIGURE 5
Coupling of Five Process Models That Describe Hourly Carbon, Water, and Chemical Dynamics in the Soil-Plant-Litter System
From Reference 3

Mass flow of solutes from the soil into the roots is simulated by the submodel DIFMAS and the transport and accumulation of solutes in vegetation and litter is simulated by the submodel DRYADS. These last two submodels can simulate effects of toxic gases and vapors, such as SO_2, as well as heavy metals.

A major drawback of the UTM arrangements is that they are restricted to substances that are conserved (i.e., metals and other inorganics). Models designed to overcome this drawback are discussed below.

MCEEA

Another site-specific model is the Multimedia Contaminant Environmental Exposure Assessment (MCEEA) method (5) developed by Battelle Pacific Northwest Laboratories for the Department of Energy to evaluate the release of radionuclides from low-level waste disposal sites. It has an integral plant growth component (BIOTRAN), as does UTM, but differs in that it has its own generator of the meteorological data it requires. Precipitation, daily temperature, and insolation are generated stochastically by random selection of parameter values from a normal distribution constructed from the long-term measured average value and variances for each parameter. The values are then used by the Agricultural Runoff Management (ARM) Model, another EPA variant of the Stanford Watershed model.

The ARM model continuously simulates the hydrodynamic response of the watershed to the meteorological conditions,

i.e., soil erosion, pollutant adsorption, removal, and decay. The data from ARM are used by the one-dimensional dynamic kinetic wave (DKWAV) model, which simulates stream hydraulics. TODAM, a one-dimensional version of SERATRA, handles the water chemistry, including transport, deposition, and scouring for three size classes of sediment. It also simulates the advection and diffusion/dispersion of both sorbed and dissolved contaminants, adsorption/desorption of dissolved pollutants by sediments, decay, deposition/resuspension of sorbed pollutants from the river bed, as well as degradation of dissolved pollutants via hydrolysis, oxidation, photolysis, and biolysis and also volatilization. TODAM also computes changes in river bed conditions. Figure 6 shows this linkage. The data requirements of MCEEA are similar to those for the UTM.

ORGANIC CHEMICALS MODELS

In the early 1980s, several continuous, site-specific, multimedia models were developed to predict organics concentrations. Included are the Unified Transport Model for Toxic Materials (UTM-TOX) and the Air, Land, Water Analysis System (ALWAS).

UTM-TOX

The original UTM arrangement was modified by the Oak Ridge National Laboratory to handle transport and transformation of organic substances. The transformation result was the Unified Transport Model for Toxic Materials (UTM-TOX) (6). In the UTM-TOX, the modified ATM submodule incorporates dispersion of the

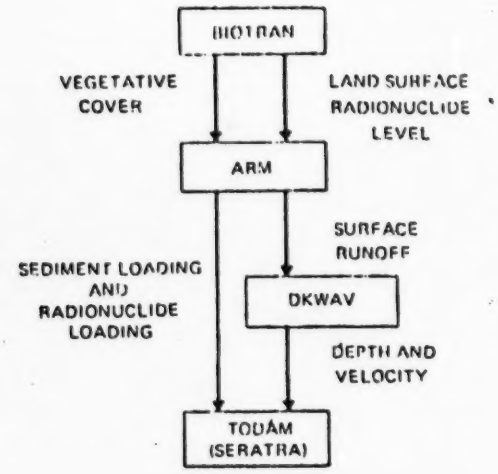

FIGURE 6
Schematic of MCEEA Model Coupling
From Reference 5

pollutant from point, line, and area sources (i.e., it now includes the consequences of an inversion lid), and both wet and dry deposition. The modified WHTM arrangement incorporates surface flow and erosion, percolation through the soil to the stream channel, and flow in the stream channel to the outfall of the watershed. Earlier versions of the UTM arrangement yielded component models that were uncoupled, for the most part. They ran serially, but separately, e.g., deposition results from the ATM were passed to a succeeding run of the WHTM. The need to treat the processes simultaneously as atmospheric loading by volatilization and deposition to the surface led to the realization that the entire set of component models should be treated as one comprehensive aggregate.

Thus, unlike the UTM, these media are coupled in the UTM-TOX in order to share common information and to serve as source terms from one medium to the next (Figure 7). The present model provides the required linkage and data to run the components of the UTM that follow. Feedback from volatilization, however, and resuspension to the atmosphere have not yet been incorporated. Differences in time scales make it difficult to effect all the intermedia linkages.

The processes added to UTM to yield UTM-TOX are similar to those in the Exposure Analysis Modeling System (EXAMS) (7). They are pollutant volatilization and biodegradation in the soil, and pollutant volatilization, biodegradation, photolysis, and hydrolysis in the water. The UTM-TOX arrangement can track a pollutant through an ecosystem and tabulates budgets for the partitioning of the pollutant and the concentration of the pollutant in many of the compartments of the ecosystem. Thus, it provides the means to assess the potential effects of a pollutant using the available data about the source of the pollutant and its chemical properties and data about the environment (4). A major remaining drawback of the UTM-TOX arrangement is that transport of chemicals has not yet been coupled to transport of sediment (i.e., it does not provide for sorption on sediment).

ALWAS

For the most part, the ALWAS was developed to link existing media-specific models into a comprehensive aggregate that could treat a range of multimedia exposure assessment problems. The

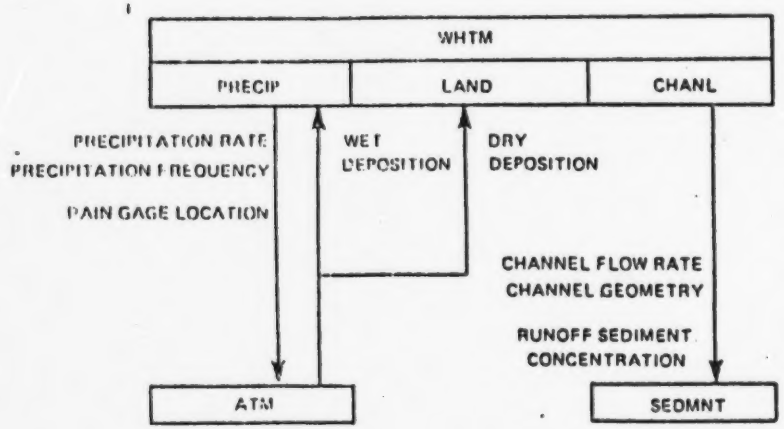

FIGURE 7
Schematic of UTM-TOX
From Reference 6

ALWAS approach is based on the premise that the processes influencing pollutant mass or concentration within each environmental medium (air, soil, water) can be combined with meteorologic and hydrologic transport mechanisms (atmospheric dispersion, runoff, erosion, stream flow, etc.) to predict the temporal and spatial distributions of pollutant concentration in each medium given appropriate information about total loading by medium. A balanced approach was desired--one that would allow consistent levels of approximation or sophistication for each component of the media manifold. The existing component or media-specific models were selected for incorporation into ALWAS according to the above criteria and include the Dispersion and Deposition of Toxics (DIDOT) model (8) for air, the Non-Point Source (NPS) model (9)

for runoff, and the Exposure Analysis Modeling System (EXAMS) (7) for water.

To facilitate and emphasize the investigation of the most important intermedia transfers of organics, an approach was adopted that minimizes feedback loops between the media-specific models. The approach avoids the need to run air, land (runoff), and aquatic models simultaneously; rather, each is run independently with the data output from one serving as data input to the others. Coupling within a given watershed as defined by aquatic and runoff models is assumed to be from air to surface (land or water) only. Because the residence time of air over a watershed is usually very short when compared to similar residence times for water or soil-related processes, the return of organics to the air from land or water (e.g., volatilization from water) is assumed to have a negligible effect on the air mass balance of a pollutant.

The processes considered important in estimating atmospheric transport and transformations include dispersion, wet and dry deposition to land or water surfaces, and chemical degradation from direct photolysis, ozone attack, OH radical attack, and RO_x radical attack. The dispersion phenomenon is applied to individual point sources (specific sources for which stack dimensions are known) and to area sources (a complex of sources to which a uniform source strength is assigned). In the general case, mass transfer to air from land and water surfaces (e.g., volatilization or wind entrainment) can also occur. Such surface-to-air transport

may be important in estimating near-surface ambient air concentrations, but, as stated earlier, it is believed to be unlikely to influence greatly the ambient concentrations in the land or the water (7).

The DIDOT model treats dispersive transport as a Gaussian phenomenon much like most air transport models do and is subject to the limitations inherent in such phenomena. Atmospheric degradation is modeled by applying aggregate pseudo-first-order kinetics to the combined processes of photolysis and the O_3, OH^{-1}, and RO_x-reactions. Inherent in this approach is the assumption that the environmental properties (e.g., the concentration of OH_3 and OH^{-1}) are relatively constant over large geographic areas of interest (e.g., rural or urban areas, watersheds, and airsheds), thus reducing the actual second-order processes to good pseudo-first-order approximations.

Compared to standard air quality models, wet and dry deposition processes in ALWAS are formulated somewhat differently. Dry deposition is estimated by accounting both for gravitational settling and surface depletion. Other air models use the source depletion method. The technical differences are described in a critique of the source depletion approach presented by Horst (10). Wet deposition processes are approximated by applying a "scavenging ratio," which is assumed to account both for vapor or air-water partitioning and for removal of particulates by rain. Finally, the DIDOT model is structured to provide loadings to land and water surfaces according to a grid network that is superimposed on the landscape.

The transport and fate of organic toxicants within and on soil systems arise from the interaction of pollutant-specific processes (e.g., degradation) and the hydrologic cycle. Transport is dominated by leaching, runoff, erosion, and sediment transport. Because pollutant transport can occur both in water and on sediment, pollutant partitioning between solution and particulate phases is necessary. The development of models to accommodate these processes has led to procedures designed for treatment of single land-use problems (e.g., agriculture, urban). However, in the general case all land uses must be included because atmospheric loading to the land surface may result from widespread movement of pollutants rather than from localized interactions within a single land use.

The land surface runoff model most compatible with the overall ALWAS design is EPA's NPS model (9). The NPS model was initially designed as an aid to the 208 water quality planning process and has been successfully applied in a number of mixed land-use watersheds (urban and rural). Two surface conditions are accommodated by the NPS: impervious surfaces like streets and roofs, and pervious surfaces like lawns, parks, and rural areas. Impervious surfaces are simulated using standard urban stormwater analysis techniques including surface accumulation of pollutants deposited from the atmosphere with subsequent washoff from precipitation-runoff. Pervious land segments generate runoff based on a continuous water balance that partitions incoming precipitation into soil moisture storage, evapotranspiration, infiltration, and surface runoff (rainfall or snowmelt). Erosion

is calculated as a function of both rainfall intensity and runoff volumes.

The NPS model simulates pollutant movement to surface water by correlation to sediment transport. That is, the sediment (referred to as "dust and dirt" in the case of impervious surfaces) predicted by the NPS model is assumed to transport a given amount of pollutant determined by the amount accumulated on the land surface and the extent to which the pollutant sorbs to sediments. This approach can lead to substantial errors, if one attempts to predict the movement of very weakly sorbed organics. For this reason, inclusion of the NPS model may limit the immediate applicability of ALWAS to hydrophobic pollutants. The NPS model is structured to accommodate loadings from the atmosphere such as those produced by the DIDOT model. Donigian and Crawford (9) discussed the NPS model in more detail.

Given appropriate organic toxicant loadings in surface water (e.g., from the NPS or DIDOT models), there remains the problem of estimating their fate and transport within selected aquatic environments. Smith et al. (11) developed a steady state, compartmentalized process model to evaluate the interactions among various aquatic fate and transport phenomena. Later Burns et al. (7) expanded this model to the EXAMS, a comprehensive organic chemical fate model based on second-order kinetic descriptions of fate processes operating at steady state within compartmentalized environments. The EXAMS is an acceptable component for ALWAS with one notable exception: its calculations

are steady state, whereas the loads calculated from the other model components are time-dependent. This limitation was overcome by the development of a time-dependent version of EXAMS for use in ALWAS.

The ALWAS "EXAMS" permits loadings from streamflow, runoff (NPS model), direct atmospheric input (DIDOT model), and any other point source effluent (either to the water column or to the benthic compartments or groundwater input). The component models in ALWAS have been selected in a way that the pollutant-specific data can be either readily obtained by laboratory measurement using existing protocols or taken from the existing literature. Hedden et al. (12) described examples and applications of ALWAS to multimedia problems.

Data Needs

Data required to perform a multimedia analysis are by no means trivial. They are, however, generally available from various inventories and national data banks. Hedden (13) has described the data needs in detail, and additional specific information requirements are described by Tucker et al. (8) in the documentation of ALWAS. The required data are of four general types: (1) environmental loading rates for sources not explicitly simulated, (2) hydrologic and meteorologic time series, (3) specific media properties, and (4) pollutant fate equilibrium and rate constants.

A major objective of multimedia modeling is to predict intermedia transfers of toxicants, but to do this, the initial

release(s) into the environment must be known. Stack emissions, stack heights, wastewater discharges, and other point sources must be identified, located, and their discharges measured or estimated. The hydrologic and meteorologic time series (wind speed and direction, inversion cap height, precipitation, stream-flow, etc.) combine to influence many of the transport and dispersion processes. Site-specific data are usually collected continuously by weather station or stream flow recordings operated by the U.S. National Weather Service and U.S. Geological Survey. Similarly, other site-specific properties (e.g., drainage areas, land use, surface water depth) that are required to define the boundary conditions and physical parameters of a model are easily obtained from the U.S. Department of Agriculture soils maps, topographic maps, planning Agency records, and other generally available sources. Finally, pollutant-specific equilibrium and kinetic rate transformation process constants must be measured or estimated using appropriate structure-activity relationships. In many cases protocols have already been developed for laboratory measurement of such data (14).

SCREENING MODELS

TOX-SCREEN

TOX-SCREEN, another model developed by the Oak Ridge National Laboratories for EPA (15), has fewer data requirements than the site-specific models. It was developed as a screening model for evaluating the potential of human exposure to chemicals. To minimize data requirements, a fixed geometry is assumed for

surface water bodies relative to atmospheric pollutant sources (point or area) and land areas, and canonical environmental data are used. The algorithms used show a trend toward simplicity, but maintain enough flexibility to describe the processes believed to be of greatest importance. The model is deliberately conservative in nature.

The estimation of the amount of intermedia pollutant flux requires that the locations and sizes of water and soil surfaces be known relative to atmospheric sources of contamination and to each other. The assumed geometry of the media sets the restraints that follow. Contaminated soil areas are adjacent to any water body present. The plume of an atmospheric pollutant source, if present, will intercept the water body at the point of maximum surface concentration, X_{max} (Figures 8 and 9). Where water bodies are not present, the land area immediately downwind from the point of maximum surface concentration is the contaminated soil area. Sizes of land and water areas are specified by the user of the model.

Concentrations of pollutant in the air, surface water, and soil reflect both direct input to any or all of the media from a specific source, or specific sources, and subsequent intermedia transport via processes such as volatilization, atmospheric deposition, and surface runoff and transformations by first-order processes. Rivers and lakes are handled in a manner similar to those of EXAMS; oceans and estuaries by models similar to those used by the Nuclear Regulatory Commission. Processes are usually

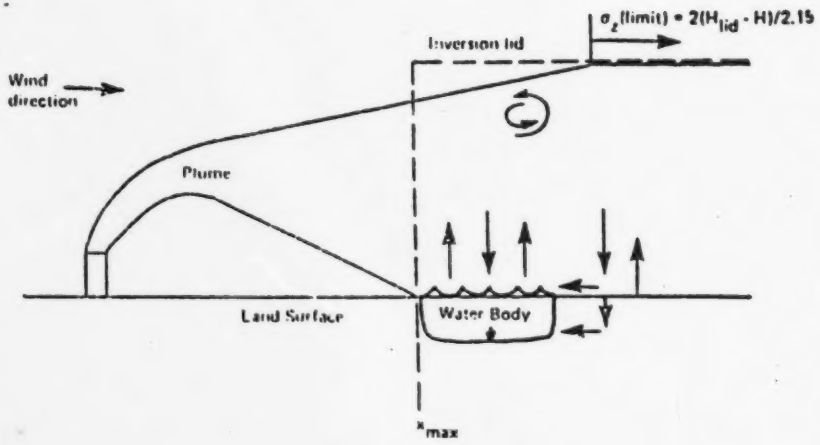

FIGURE 8
Geometry of Water Body to Stack (Plume Source) in TOX-SCREEN. The point of maximum concentration, X_{max}, is defined as the edge of the water body immediately downwind of the source. Possible pollutant movement is shown by arrows.
From Reference 15

handled explicitly using deposition velocities, rate coefficients, and mass loading parameters. The type of water bodies (i.e., river, lake, estuary, or ocean) to be simulated must be specified along with the medium to which the pollutant is directly released.

ADL Models

The ADL models, which simply describe the partitioning of a pollutant among the various media, require fewer data. Two such screening models were developed by A.D. Little (ADL) for EPA (16). One is based on the "model ecosystem" of Neeley of Dow Chemical. A set of empirical regression equations (Figure 10) was developed from the model ecosystem to estimate partitioning among air,

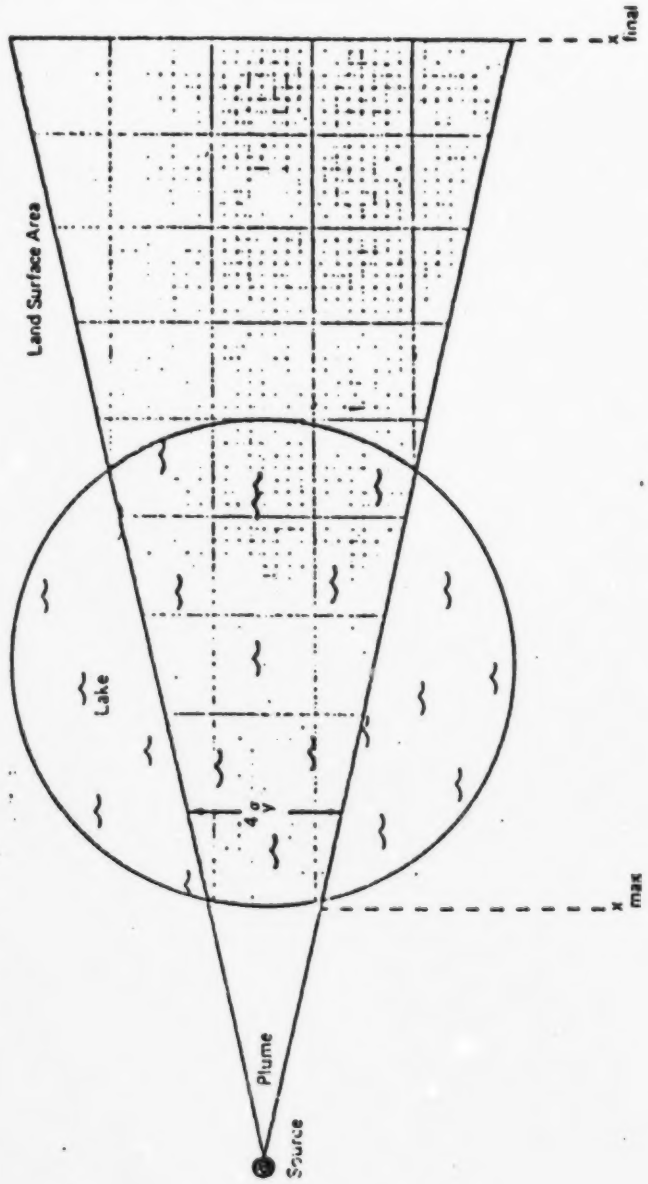

FIGURE 9
Diagram of the Air-Lake and Air-Soil Interaction Scenario Assessment in TOX-SCREEN, for a Pollutant Point Source. The shaded area indicates the zone of contamination.
From Reference 15

PERCENT IN AIR	=	00.247 (1/H) + 7.9 LOG S + 100.6
PERCENT IN WATER	=	0.054 (1/H) + 1.32
PERCENT IN SOIL	=	0.194 (1/H) - 7.65 LOG S - 1.93
LOG $t_{1/2}$	=	0.0027 (1/H) - 0.282 LOG S + 1.08
where H	=	HENRY'S LAW CONSTANT = P_{vp}/S
S	=	WATER SOLUBILITY (mM/L)
P_{vp}	=	VAPOR PRESSURE (mm Hg)
$t_{1/2}$	=	HALF-LIFE FOR CLEARANCE FROM FISH IN ECOSYSTEM (hr)

FIGURE 10
Regression Equations that
Describe the Neely Model Ecosystem
From Reference 16

water, and soil and also a half-life for clearance from fish. To use the Neely model, one only needs the parameters because the environment is set and the partitioning among the various media is the model output.

The other ADL model is based on the fugacity model of Mackay. A predetermined environment with air, land, water, suspended solids, and biota compartments is used. A tiered application approach is suggested by Mackay. The data requirements are chemical-specific, increasing in number as the tier increases:

> Level I considers the equilibrium partitioning of an organic chemical in a static environment with specified subcompartments (e.g., air, water, soil, biota) and no degradation or transport. The method requires specification of minimal environmental data (volumes, sediment and biota "concentrations," temperature, etc.), plus the amount of chemical released into the model environment and a small number of chemical-specific parameters to be used to calculate a "fugacity capacity constant" Z, which is related to fugacity f and compartment concentration C, by the formula C = Zf.
>
> Level II allows both pollutant transport into and out of the model environment and degradation by first-order processes. Concentrations in specified subcompartments, removal rates, and an overall lifetime for the chemical in the model environment are calculated by the basic fugacity approach.
>
> Level III improves upon level II by allowing a steady-state input of the chemical into any subcompartment as well as non-instantaneous intercompartment transfers (e.g., volatilization). Otherwise, all output remains the same as for the lower tiers.

ENPART

ENPART, the last screening model to be discussed, was developed by the EPA Office of Toxic Substances (17). It is a partitioning model, based on the work of Mackay. It partitions a pollutant between air and water and air and soil compartments.

Relatively extensive chemical-specific data are required along with a limited amount of environmental data. The chemical data are similar to those required by the previously described models. The environmental data needed include soil bulk density, suspended sediment concentration, biota concentration, lipid fraction, bottom sediment bulk density, and also some dynamic input information.

ENPART, UTM-TOX, and TOX-SCREEN and several single-media models are included by EPA in a developmental package that provides several levels of modeling ranging from fairly sophisticated and data intensive to those requiring a minimum amount of data. This

package, called Graphical Exposure Modeling System (GEMS), also includes 1980 Census data down to enumeration district, plus other on-line data bases.

SUMMARY

Several multimedia fate and transport models have been described. They basically fall into three classes: continuous (dynamic) site-specific models; generic (non-site-specific) screening models; and simple equilibrium partitioning screening models. The hydrologic components of site-specific models are all based on the Stanford Watershed Model. They all link existing single media models (e.g., air, land, water), but are not yet completely coupled. For each site-specific model, there are plans to eventually allow for feedback between media.

The screening models take a variety of approaches, are much less data intensive than the site-specific models, and are mainly used to identify the media in which further efforts should be directed.

As time goes on, many more multimedia methods will undoubtedly be developed and applied to problems of EPA concern. A major impediment to widespread use that needs to be overcome is a general lack of adequate data to test, calibrate, implement, and use the various models, particularly the more sophisticated ones. Many of the necessary monitoring data are lacking or inappropriate for modeling use, as are the needed chemical and environmental data. Therefore, modeling objectives will need to be considered in the planning of improved and expanded monitoring

efforts. Better communication between users and modelers needs to be established (18). Bases of chemical and environmental data of known quality need to be developed, along with more structure-activity relationships for predicting chemical properties. In short, the widespread use of multimedia models will depend on the availability of data rather than on the availability of a model.

REFERENCES

1. Hoffman, F.O., D.L. Shaeffer, C.W. Miller, and C.T. Garten, Jr. 1978. Proceedings of a workshop on the evaluation of models used for the environmental assessment of radionuclide releases. Oak Ridge National Laboratory, CONF-770901. Oak Ridge, Tennessee.

2. Meadows, D.H., D.L. Meadows, J. Randers, and W.W. Behrens. 1972. The limits to growth. Washington:Signet Books.

3. Munro, J.R., R.J. Luxmoore, C.L. Begovich, K.R. Dixon, A.P. Watson, M.R. Patterson, and D.R. Jackson. 1977. Transport model to predict the movement of Pb, Cd, Zn, Cu, and S through a forested watershed. In Disposal of residues on land, 45-58. U.S. Environmental Protection Agency, Washington, D.C.

4. Huff, D.D., R.J. Luxmoore, J.B. Mankin, and C.L. Begovich. 1977. TEHM: A terrestrial ecosystem hydrology model. Oak Ridge National Laboratory, ORNL/NSF/EWATL-27. Oak Ridge, Tennessee.

5. Onishi, Y., G. Whelan, and R.L. Skaggs. 1982. Development of a multimedia radionuclide exposure assessment methodology for low-level waste management. Battelle Pacific Northwest Laboratory, PNL-3370. Richland, Washington.

6. Patterson, M.R., T.J. Sworski, A.L. Sjoreen, M.G. Browman, C.C. Coutant, D.M. Hetrick, B.D. Murphy, and R.J. Raridon. 1982. A user's manual for UTM-TOX, a unified transport model. Prepared under IAG No. AD-89-F-1-399-0 by Oak Ridge National Laboratory for the U.S. Environmental Protection Agency, Washington, D.C.

7. Burns, L.A., D.M. Cline, and R.R. Lassiter. 1982. Exposure analysis modeling system (EXAMS): User manual and system documentation. U.S. Environmental Protection Agency, EPA-600/3-82-023. Athens, Georgia.

8. Tucker, W.A., A.Q. Eschenroeder, and G.C. Magil. 1982. Air, land, water analysis system (ALWAS): A multimedia model for assessing the effects of airborne toxic substances on surface water quality. U.S. Environmental Protection Agency, Athens, Georgia. In preparation.

9. Donigian, A.S., and N.H. Crawford. 1976. Modeling nonpoint pollution from the land surface. U.S. Environmental Protection Agency, EPA-600/3-76-083. Athens, Georgia.

10. Horst, T.W. 1977. A surface depletion model for deposition from a Gaussian plume. Atmos. Environ. 11:41-46.

11. Smith, J.H., W.R. Mabey, N. Bohonos, B.R. Holt, S.S. Lee, T.W. Chou, D.C. Bomberger, and T. Mill. 1977. Environmental pathways of selected chemicals in freshwater systems. Part I: Background and experimental procedures. U.S. Environmental Protection Agency, EPA-600/7-77-113. Athens, Georgia.

12. Hedden, K.F., L.A. Mulkey, and W.A. Tucker. 1982. Application of multimedia exposure assessment to drinking water. Environ. Monitor. Assess. 2:57-69.

13. Hedden, K.F. 1981. Multimedia exposure assessment model data needs. In 1981 Conference on environmental engineering, ed. F.M. Saunders, 150-158. New York:American Society of Civil Engineers.

14. Mill, T., W.R. Mabey, D.C. Bromberger, T.W. Chou, D.G. Hendry, and J.H. Smith. 1982. Laboratory protocols for evaluating the fate of organic chemicals in air and water. U.S. Environmental Protection Agency, EPA-600/3-82-002. Athens, Georgia.

15. McDowell-Boyer, L.M., and D.M. Hetrick. 1982. A multimedia screening-level model for assessing the potential fate of chemicals released to the environment. Oak Ridge National Laboratory, ORNL/TM8334. Oak Ridge, Tennessee.

16. Lyman, W.J. 1981. Prediction of chemical partitioning in the environment: An assessment of two screening models. Prepared under Contract 68-01-5949 for the U.S. Environmental Protection Agency, Washington, D.C.

17. Wood, W.P., I.A. Nold, J. Lefler, and J.O. Pilotte. 1982. Environmental partitioning model. U.S. Environmental Protection Agency, Draft Report. Washington, D.C.

18. Miller, C. 1978. Exposure assessment modeling: A state-of-the-art review. U.S. Environmental Protection Agency, EPA-600/3-78-065. Athens, Georgia.

DISCUSSION

Casey Jason, Environmental Protection Agency: Which of the EPA models has actually been tested at this point--the actual measurements, the limits of the measurements--and has actually been shown to be a valid model?

Dr. Hedden: The one that has the most extensive testing is the UTM, which is approximately 10 years old. It has been tested on a number of watersheds, varying from a couple hundred acres to a couple hundred square miles. That relates to UTM-TOX.

The hydrologic transport side of the two are essentially the same, but one looks at trace metals and the other at organics. None of these has had extensive testing. The Stanford Watershed Model, on which the more site-specific of these, the land and runoff side, are based, has had extensive testing on the transport side. So, portions of these are fairly well tested, portions of them are not, but all except for the UTM are of quite recent development, basically just coming out within the last year or two.